Neural Path Features and Neural Path Kernel : Understanding the role of gates in deep learning

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Abstract

Rectified linear unit (ReLU) activations can also be thought of as *gates*, which, either pass or stop their pre-activation input when they are *on* (when the pre-activation input is positive) or *off* (when the pre-activation input is negative) respectively. DNNs with ReLU activations has many gates, and the on/off status of each gate changes across input examples as well as network parameters. For a given input example, only a subset of gates are *active*, i.e., on. Thus for that particular input example, only the sub-network of weights connected to these active gates is responsible for producing the output. Input examples that are close to one another will have similar set of active gates. While at randomised initialisation, the active sub-network corresponding to a given input example is random, during training, as the network parameters are learnt, the sub-network is also learnt, and potentially holds very valuable information.

Our aim is to understand the role of the gates, and the dynamics of gate activity during training in DNNs. The gate activity, i.e., the on/off state of the gates of a given input is captured in a novel *neural path feature* (NPF), and the weights of the DNN are encoded in a novel *neural path value* (NPV), and the output of network is expressed as an inner product of NPF and NPV. As a result, the gradient of the output contains two components, each separately responsible for learning the NPFs and NPVs. We show the *neural path kernel* associated with the NPF is a fundamental quantity that characterises the information stored in the gates of a DNN. We show via experiments that in standard DNNs with ReLU activations NPFs are learnt during training and such learning is key for generalisation. Furthermore, NPFs and NPVs can be learnt in two separate networks and such learning also generalises well in experiments. In our experiments on CIFAR-10 and MNIST datasets, we observe that almost all the information learnt by a DNN with ReLU activations is stored in the gates - a novel observation that underscores the need to further investigate the role of gating in DNNs.

1 Introduction

Understanding optimisation and generalisation in deep neural networks (DNNs) trained using first-order method such as gradient descent (GD) is an important problem in machine learning. Despite having a non-convex loss surface, GD achieves zero training error in over-parameterised DNNs where the number of parameters exceeds the size of the dataset. Interestingly, **?** demonstrated that practical DNNs have enough capacity to achieve zero training loss with even random labelling of standard datasets such as MNIST and CIFAR. However, when trained with true labels, such networks achieve zero training error and also exhibit good performance on test data.

In what follows ,we denote the dataset by $(x_s, y_s)_{s=1}^n \in \mathbb{R}^{d_{in}} \times \mathbb{R}$, and the parameters of the network by $\Theta \in \mathbb{R}^{d_{net}}$, the network output for an input $x \in \mathbb{R}^{d_{in}}$ by $\hat{y}_\Theta(x)$.

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Some of the recent works (**? ? ? ?**) on this problem have made use of the *neural tangent features* (NTFs) and the *trajectory based analysis*, which we describe in brief. The NTF of an input $x \in \mathbb{R}^{d_{in}}$ is defined as $\psi_{x,\Theta} = (\partial_\theta \hat{y}_\Theta(x), \theta \in \Theta) \in \mathbb{R}^{d_{net}}$[1], i.e., the gradient of the network output with respect to the weights. By collecting the NTFs of all the inputs examples in the dataset, we can form the NTF matrix $\Psi = (\psi_{x_s,\Theta}, s \in [n]) \in \mathbb{R}^{d_{net} \times n}$[2]. The trajectory based analysis looks at the dynamics of the error $e_t = (\hat{y}_{\Theta_t} - y_s, s \in [n]) \in \mathbb{R}^n$. For a small enough step-size $\alpha_t > 0$ of the GD procedure, the error dynamics is given by:

$$e_{t+1} = e_t - \alpha_t K_{\Theta_t} e_t, \tag{1}$$

where $K_{\Theta_t} \in \mathbb{R}^{n \times n}$ is the *neural tangent kernel* (NTK) matrix give by $K_\Theta = \Psi_\Theta^\top \Psi_\Theta$. Thus, the spectral properties, and in particular, $\rho_{\min}(K_{\Theta_t})$ the minimum eigenvalue of K_{Θ_t} dictates the rate of convergence. Under randomised initialisation, and in the limit of infinite width an interesting property emerges: the parameters of the DNN deviate very little during training, i.e. $\Theta_t \approx \Theta_0$. In particular, $K_{\Theta_t} \approx K_{\Theta_0}, K_{\Theta_0} \to K^{(d)}$, i.e., the NTK stays almost constant through training and the NTK matrix at initialisation K_{Θ_0} converges to a deterministic matrix $K^{(d)}$ (see **??** for exact expression of $K^{(d)}$. Thus in the 'large-width' regime, zero training error can be achieved if $\rho_{\min}(K^{(d)}) > 0$ which holds as long as the training data is not degenerate (**? ?**). In the 'large-width' regime, **?** show that the fully trained DNN is equivalent to kernel regression with $K^{(d)}$. Hence, a trained DNN enjoys the generalisation ability of its corresponding $K^{(d)}$ matrix in the 'large-width' regime. **?** show that in the 'large-width' regime, the DNN is almost a linear learner with the random NTFs, and showed a generalisation bound in the form of $\tilde{\mathcal{O}}\left(d \cdot \sqrt{y^\top K^{(d)} y/n}\right)$[3], where $y = (y_s, s \in [n]) \in \mathbb{R}^n$ is the labelling function.

Research Gap I (Feature Learning): In the 'large-width' i.e., fixed NTF/NTK regime, the DNNs are linear learner using the random NTFs at random initialisation. This implies that there is little or no feature learning. Is this true for standard DNNs with finite width as well?
Research Gap II (Finite vs Infinite): **?** note that, while pure-kernel methods based on the limiting NTK (i.e., $K^{(d)}$) outperform other state-of-the-art kernel methods, the finite width DNNs (CNNs) still outperform their NTK (CNTK) [4] counterpart. Can we explain this gap?

2 Path-View: Capturing Feature Learning

In this paper, we take the 'path-view': the output of a DNN is obtained as a summation of the contribution of individual paths, which is possible due to the gating property of the ReLU activations. Each path contains gates and weights, and the contribution of a path is the product of the gates and the weights in the path. While the weights remain the same the role of gates in a DNN, by splitting them into i) *active* gates and ii) *sensitive* gates.

• Active Gates/Paths: For each input example, only a subset of the gates are active, i.e., *on*. For each input example, there is a corresponding active sub-network comprising of active gates and the paths passing through the active gates. This active sub-network can be said to hold the memory for a given input, i.e., only those active paths that pass through the active gates contribute to the output.

• Sensitive Gates/Paths: For each input example, a sub-set of have gates have their pre-activation input to be near 0. Such gates are called sensitive gates, since they can flip from 0 to 1 or vice-versa based on gradient information. Thus, by tuning such sensitive gates, gradient descent learns the right active sub-network for each input in the dataset.

In what follows, we formally define a path, the neural path feature (NPF) which captures the states of the gates, and the neural path value (NPV) which encodes the weights of a DNN. This enable us to express the output $\hat{y}_\Theta(x)$ as an inner-product of NPF and NPV, and we 'plug-in' this output expression in $\partial_\theta \hat{y}_\Theta(x)$. We obtain expanded expressions for the NTF and NTK that contain the NPFs, NPVs and the gradients of NPFs and NPVs.

[1]Here $\partial_\theta(\cdot)$ stands for $\frac{\partial(\cdot)}{\partial\theta}$
[2]$[n] = \{1, \ldots, n\}$
[3]$a_t = \mathcal{O}(b_t)$ if $\limsup_{t\to\infty} |a_t/b_t| < \infty$, and $\tilde{\mathcal{O}}(\cdot)$ is used to hide logarithmic factors in $\mathcal{O}(\cdot)$.
[4]CNTK: Convolutional Neural Tangent Kernel, the NTK for CNNs

2.1 Paths and Gates

We denote by $\Theta(l, j, i)$ the weight connecting the j^{th} hidden unit of layer $l-1$ to the i^{th} hidden unit of layer $l \in [d]$.

Input Layer	$z_{x,\Theta}(0)$	$=$	x
Pre-Activation	$q_{x,\Theta}(l,i)$	$=$	$\Theta(l,\cdot,i)^\top z_{x,\Theta}(l-1), l \in [d-1], i \in [w]$
Gating Values	$G_{x,\Theta}(l,i)$	$=$	$\gamma(q_{x,\Theta}(l,i)), l \in [d-1], i \in [w]$
Hidden Layer	$z_{x,\Theta}(l,i)$	$=$	$\chi(q_{x,\Theta}(l,i)) = q_{x,\Theta}(l,i) \cdot G_{x,\Theta}(l,i), l \in [d-1], i \in [w]$
Final Output	$\hat{y}_\Theta(x)$	$=$	$\Theta(d)^\top z_{x,\Theta}(d-1)$

Table 1: Here $\Theta(1) \in \mathbb{R}^{w \times d_{in}}, \Theta(l) \in \mathbb{R}^{w \times w}, \forall l \in \{2, \ldots, d-1\}, \Theta(d) \in \mathbb{R}^{w \times 1}$.

Paths: A path starts from an input node, passes through exactly one weight (and one hidden node) in each layer and ends at the output node. We have a total of $P = d_{in} w^{(d-1)}$ paths. Let us say that an enumeration of the paths is given by $[P] = \{1, \ldots, P\}$. Let $\mathcal{I}_l \colon [P] \to [w], l = 0, \ldots, d-1$ provide the index of the hidden unit through which a path p passes in layer l (with the convention that $\mathcal{I}_d(p) = 1, \forall p \in [P]$).

Gates: We consider two kinds of gates namely, i) ReLU and ii) soft-ReLU. Let $q \in \mathbb{R}$ be a pre-activation input. In the case of ReLU, the gating and activations are given by $\gamma_r(q) = \mathbb{1}_{\{q>0\}}$ and $\chi_r(q) = q \cdot \gamma_r(q)$. In the case of soft-ReLU, the gating and activations are given by $\gamma_{sr}(q) = \frac{1}{(1+\exp(-\beta \cdot q))}, \beta > 0$, and the activation is given by $\chi_{sr}(q) = q \cdot \gamma_{sr}(q)$.

Remark: In the case of ReLU, the derivative of the gate is almost surely 0, the role of the sensitive gates cannot be captured. This can be remedied by considering the soft-ReLU gates, where, the derivative of the gating with respect to the pre-activation is given by $\partial_q \gamma_{sr}(q) = \frac{\beta}{(1+\exp(\beta \cdot q))(1+\exp(-\beta \cdot q))}$.

2.2 Neural Path Feature, Neural Path Value and Network Output

The activity of a path p for an input $x \in \mathbb{R}^{d_{in}}$ by

$$A_\Theta(x,p) \stackrel{def}{=} \Pi_{l=1}^{d-1} G_{x,\Theta}(l, \mathcal{I}_l(p)) \tag{2}$$

The *neural path feature* (NPF) of an input $x \in \mathbb{R}^{d_{in}}$ is given by

$$\phi_{x,\Theta} \stackrel{def}{=} (x(\mathcal{I}_0(p)) A_\Theta(x_s, p), p \in [P]) \in \mathbb{R}^P, \tag{3}$$

where, for a path p, $\mathcal{I}_0(p)$ is the input node at which the path starts, and $A_\Theta(x,p)$ is its activity.

The *neural path value* (NPV) if given by

$$v_\Theta \stackrel{def}{=} \left(\Pi_{l=1}^{d} \Theta(l, \mathcal{I}_{l-1}(p), \mathcal{I}_l(p)), p \in [P]\right) \in \mathbb{R}^P \tag{4}$$

Note that, in the case of DNN with ReLU activations, the following hold:

1. The NPFs are *positively homogenous*, i.e., $\phi_{cx,\Theta} = c\phi_{x,\Theta}, \forall c > 0, x \in \mathbb{R}^{d_{in}}$.

2. For a path p, its co-ordinate $\phi_{x,\Theta}(p)$ is 0 if any one of the gates in the path is off, and is equal to the signal at the input node if all the gates in the path are on.

Proposition 2.1. *The output of the network can be written as an inner product of the NPF and NPV as below:*

$$\hat{y}_\Theta(x) = \langle \phi_{x,\Theta}, v_\Theta \rangle = \sum_{p \in [P]} x(\mathcal{I}_0(p)) A_\Theta(x,p) v_\Theta(p) \tag{5}$$

Define the vector of outputs $\hat{y}_\Theta \stackrel{def}{=} (\hat{y}_\Theta(x_s), s \in [n]) \in \mathbb{R}^n$, and the NPF matrix $\Phi_\Theta = (\phi_{x_s,\Theta}, s \in [n]) \in \mathbb{R}^{P \times n}$. Then the input-output relationship of a DNN in vector form is given by:

$$\hat{y}_\Theta = \Phi_\Theta^\top v_\Theta \tag{6}$$

Thus gradient descent on $\Theta \in \mathbb{R}^{d_{net}}$ changes both quantities Φ_Θ and v_Θ, of which, Φ_Θ captures the information in the gates. Further, the NPV is a P dimensional quantity, however, loosely speaking, its 'degrees of freedom' is restricted by its parameter Θ, whose dimension is d_{net}.

2.3 Neural Tangent Feature and Kernel

Recall that the *neural tangent feature* (NTF) of an input $x \in \mathbb{R}^{d_{in}}$ is given by $\psi_{x,\Theta} = (\partial_\theta \hat{y}_\Theta(x), \theta \in \Theta) \in \mathbb{R}^{d_{net}}$. By 'plugging' the expression for $\hat{y}_\Theta(x)$ in $\partial_\theta \hat{y}_\Theta(x)$, we have

$$\begin{aligned}\partial \hat{y}_\Theta(x) &= \underbrace{\langle \phi_{x,\Theta}, \partial v_\Theta \rangle}_{\text{value derivative}} + \underbrace{\langle \partial \phi_{x,\Theta}, v_\Theta \rangle}_{\text{feature derivative}} \\ &= \sum_{p\in[P]} x(\mathcal{I}_0(p)) A_\Theta(x,p) \partial v_\Theta(p) + \sum_{p\in[P]} x(\mathcal{I}_0(p)) \partial A_\Theta(x,p) v_\Theta(p)\end{aligned} \tag{7}$$

Note that due to the $A_\Theta(x,p)$, only active paths (those passing through active gates) contribute to the value derivative, and due to the $\partial A_\Theta(x,p)$, only sensitive paths (those passing through sensitive gates) contribute to the feature derivative.

Proposition 2.2. *Let p be a path, and let $\theta \in \Theta$ be an arbitrary weight belonging to layer $l' \in [d]$ such that $\theta = \Theta(l', i, j)$. Then $\partial_\theta v_\Theta(p) = 0$ if the path does not pass through the weight, and $\partial_\theta v_\Theta(p) = \Pi_{l\neq l', l=1}^{d} \Theta(l, \mathcal{I}_{l-1}(p), \mathcal{I}_l(p))$.*

Proposition 2.3. *Let p be a path, and let $\theta \in \Theta$ be an arbitrary weight, then $\partial_\theta A_\Theta(x,p) = \sum_{l=1}^{d} \partial G_{x,\Theta}(l) \Pi_{l'\neq l} G_{x,\Theta}(l')$*

From (7) we have $\psi_{x,\Theta} = \psi^{\text{V}}_{x,\Theta} + \psi^{\text{F}}_{x,\Theta}$, where ψ^{V} and ψ^{F} denote the value and feature gradients given by $\psi^{\text{V}}_{x,\Theta} = (\langle \phi_{x,\Theta}, \partial_\theta v_\Theta \rangle, \theta \in \Theta) \in \mathbb{R}^{d_{net}}$ and $\psi^{\text{F}}_{x,\Theta} = (\langle \partial_\theta \phi_{x,\Theta}, v_\Theta \rangle, \theta \in \Theta) \in \mathbb{R}^{d_{net}}$ respectively.

The *neural tangent kernel* matrix is given by $K_\Theta(s,s') = \langle \psi_{x_s,\Theta}, \psi_{x_{s'},\Theta} \rangle, s, s' \in [n]$ and can be further decomposed as:

$$K_\Theta = K^{\text{V}}_\Theta + K^{\text{F}}_\Theta + K^{\text{CROSS}}_\Theta, \tag{8}$$

where $K^{\text{V}}_\Theta(s,s') = \langle \psi^{\text{V}}_{x_s,\Theta}, \psi^{\text{V}}_{x_{s'},\Theta} \rangle$ is the kernel corresponding to learning NPVs, $K^{\text{F}}_\Theta(s,s') = \langle \psi^{\text{F}}_{x_s,\Theta}, \psi^{\text{F}}_{x_{s'},\Theta} \rangle$ is the kernel corresponding to learning NPFs, and $K^{\text{CROSS}}_\Theta(s,s') = \langle \psi^{\text{V}}_{x_s,\Theta}, \psi^{\text{F}}_{x_{s'},\Theta} \rangle + \langle \psi^{\text{F}}_{x_s,\Theta}, \psi^{\text{V}}_{x_{s'},\Theta} \rangle$ is a symmetric matrix of the cross-terms in the expansion of $K_\Theta(s,s')$.

2.4 Gradient Descent Dynamics With Neural Path Feature Learning

Proposition 2.4. *For small step-size $\alpha_t \to 0$, the gradient descent dynamics with NPF learning can be given by:*

Parameter Dynamics	$\dot{\Theta}_t$	$=$	$-\sum_{s=1}^{n} \psi_{x_s,\Theta_t} e_t(s) = \sum_{s=1}^{n} (\psi^{\text{V}}_{x_s,\Theta_t} + \psi^{\text{F}}_{x_s,\Theta_t}) e_t(s)$
NPF Dynamics	$\dot{\phi}_{x_s,\Theta_t}(p)$	$=$	$x(\mathcal{I}_0(p)) \sum_{\theta\in\Theta} \partial_\theta A_{\Theta_t}(x_s,p) \dot{\theta}_t, \forall p \in [P], s \in [n]$
NPV Dynamics	$\dot{v}_{\Theta_t}(p)$	$=$	$\sum_{\theta\in\Theta} \partial_\theta v_{\Theta_t}(p) \dot{\theta}_t, \forall p \in [P]$
Error Dynamics	$\dot{e}_t$	$=$	$-K_{\Theta_t} e_t$, where $K_\Theta = K^{\text{V}}_\Theta + K^{\text{F}}_\Theta + K^{\text{CROSS}}_\Theta$

3 Decoupling NPF and NPV

In the previous section, we wrote down the gradient descent dynamics, wherein, both the NPVs and the NPFs are learnt during training. In order to better understand the roles of the NPVs and NPFs, we separate them out in this section. This separation can be achieved by a deep gated network (see Figure 1 below for details) having two networks of identical architecture namely i) a feature network parameterised by $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$, that holds gating information, and hence the NPFs and ii) a value network that holds the NPVs parameterised by $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$. In what follows, we denote by $\Theta^{\text{DGN}} = (\Theta^{\text{F}}, \Theta^{\text{V}}) \in \mathbb{R}^{2d_{net}}$ the combined weights of the DGN. Having separated the NPV and the NPF, we setup the following two problems:

1. Fixed NPF (FNPF): Here, we learn the relation $\hat{y}_{\Theta^{\text{DGN}}} = \Phi^\top_{\Theta^{\text{F}}_0} v_{\Theta^{\text{V}}}$, where only Θ^{V} is trained using gradient descent, while, $\Theta^{\text{F}}_t = \Theta^{\text{F}}_0, \forall t \geq 0$ is non-trainable. Thus, $\Phi_{\Theta^{\text{F}}_0} \in \mathbb{R}^{P\times n}$, which is a fixed NPF matrix.

2. Decoupled NPF Learning (DNPFL): Here, we learn the relation $\hat{y}_{\Theta^{\text{DGN}}} = \Phi^\top_{\Theta^{\text{F}}} v_{\Theta^{\text{V}}}$, where the we learn both Θ^{F} and Θ^{V}.

In what follows, we present the DGN framework, followed by which, we write down the gradient descent dynamics for FNPF and DNPFL. We then show that the *neural path kernel* associated with the NPFs characterises the information stored in the gates of a DNN.

3.1 Deep Gated Networks

Layer	Feature Network (NPF)	Value Network (NPV)
Input	$z^{\text{F}}_{x,t}(0) = x$	$z^{\text{V}}_{x,t}(0) = x$
Activation	$q^{\text{F}}_{x,t}(l) = \Theta^{\text{F}}_t(l)^\top z^{\text{F}}_{x,t}(l-1)$	$q^{\text{V}}_{x,t}(l) = \Theta^{\text{V}}_t(l)^\top z^{\text{V}}_{x,t}(l-1)$
Hidden	$z^{\text{F}}_{x,t}(l) = \chi^{\text{F}}\left(q^{\text{F}}_{x,t}(l)\right)$	$z^{\text{V}}_{x,t}(l) = q^{\text{V}}_{x,t}(l) \odot G_{x,t}(l)$
Output	$\hat{y}^{\text{F}}_t(x) = \Theta^{\text{F}}_t(d)^\top z^{\text{F}}_{x,t}(d-1)$	$\hat{y}^{\text{V}}_t(x) = \Theta^{\text{V}}(d)^\top z^{\text{V}}_{x,t}(d-1)$
Gating Values: $G_{x,t}(l) = \gamma_r\left(q^{\text{F}}_{x,t}(l)\right)$ or $G_{x,t}(l) = \gamma_{sr}\left(q^{\text{F}}_{x,t}(l)\right)$		

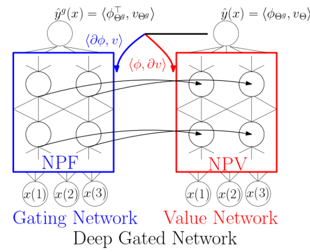

Figure 1: Deep gated network (DGN) setup.

Note that, the feature network uses χ^{F} as the activation function, which can be a standard ReLU activation, i.e., $\chi^{\text{F}} = \chi_r$. The pre-activations $q^{\text{F}}_{x,t}(l)$ of layer $l \in [d-1]$ from the feature network are used to derive the gating values $G_{x,t}(l)$ of layer $l \in [d-1]$. The gating values can be obtained from either a ReLU gate γ_r or a soft-ReLU gate γ_{sr}. The process of separating the NPFs and the NPVs decouples the value and the feature gradients. In a DGN, the value gradient $\psi^{\text{V}}_{x,\Theta^{\text{DGN}}}$ flows through the value network and the feature gradient $\psi^{\text{F}}_{x,\Theta^{\text{DGN}}}$ flows through the feature network.

3.2 Gradient Dynamics of FNPF and DNPFL

Proposition 3.1 (FNPF)**.** *The gradient dynamics is given by*

Parameter Dynamics	$\dot{\Theta}^{\text{V}}_t$	$=$	$-\sum_{s=1}^n \psi^{\text{V}}_{x,\Theta^{\text{DGN}}_t} e_t(s),\ \dot{\Theta}^{\text{F}}_t = 0$
NPF Dynamics	$\dot{\phi}_{x_s,\Theta^{\text{F}}_t}(p)$	$=$	$0, \forall p \in [P], s \in [n]$
NPV Dynamics	$\dot{v}_{\Theta^{\text{V}}_t}(p)$	$=$	$\sum_{\theta^{\text{V}} \in \Theta^{\text{V}}} \partial_{\theta^{\text{V}}} v_{\Theta^{\text{V}}_t}(p)\dot{\theta}^{\text{V}}_t, \forall p \in [P]$
Error Dynamics	$\dot{e}_t$	$=$	$-\left(K_{\Theta^{\text{DGN}}_t}\right) e_t$, where $K_{\Theta^{\text{DGN}}} = K^{\text{V}}_{\Theta^{\text{DGN}}}$

Proposition 3.2 (DNPFL)**.** *The gradient dynamics is given by*

Parameter Dynamics	$\dot{\Theta}^{\text{V}}_t$	$=$	$-\sum_{s=1}^n \psi^{\text{V}}_{x,\Theta^{\text{DGN}}_t} e_t(s),\ \dot{\Theta}^{\text{F}}_t = -\sum_{s=1}^n \psi^{\text{F}}_{x,\Theta^{\text{DGN}}_t} e_t(s)$
NPF Dynamics	$\dot{\phi}_{x_s,\Theta^{\text{F}}_t}(p)$	$=$	$x(\mathcal{I}_0(p)) \sum_{\theta^{\text{F}} \in \Theta^{\text{F}}} \partial_{\theta^{\text{F}}} A_{\Theta^{\text{F}}_t}(x_s, p)\dot{\theta}^{\text{F}}_t, \forall p \in [P], s \in [n]$
NPV Dynamics	$\dot{v}_{\Theta^{\text{V}}_t}(p)$	$=$	$\sum_{\theta^{\text{V}} \in \Theta^{\text{V}}} \partial_{\theta^{\text{V}}} v_{\Theta^{\text{V}}_t}(p)\dot{\theta}^{\text{V}}_t, \forall p \in [P]$
Error Dynamics	$\dot{e}_t$	$=$	$-\left(K_{\Theta^{\text{DGN}}_t}\right) e_t$, where $K_{\Theta^{\text{DGN}}} = K^{\text{V}}_{\Theta^{\text{DGN}}} + K^{\text{F}}_{\Theta^{\text{DGN}}}$

4 Measure of Information in Gates: Neural Path Kernel

Suppose we have a DNN with parameter $\bar{\Theta} \in \mathbb{R}^{d_{net}}$, and we want to measure the information in the gates of this DNN. One way to accomplish this task is to set $\Theta^{\text{F}}_t = \bar{\Theta}, \forall t \geq 0$ in the DGN framework and train $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$ using gradient, i.e., use the fixed NPF obtained from $\bar{\Theta}$ and learn only the NPVs. The generalisation performance of this FNPF learner can then be used as a measure of the information in the gates of the DNN with parameter $\bar{\Theta}$.

We now present a result that states that, in the limit of 'large-width', the performance of the FNPF learning tied down to its associated *neural path kernel* (NPK). We then discuss the special structure of the NPK, wherein, the similarity of the sub-networks for different input examples plays a critical role.

Assumption 1 (Independent Initialisation). *(i)* $\Theta^V_0 \in \mathbb{R}^{d_{net}}$ *is statistically independent of* Θ^F_0*, (ii)* Θ^V_0 *are sampled i.i.d from a distribution such that for any* $\theta^V_0 \in \Theta^V_0$*, we have* $\mathbb{E}\left[\theta^V_0\right] = 0$*, and* $\mathbb{E}\left[(\theta^V_0)^2\right] = \sigma^2$*, and* $\mathbb{E}\left[(\theta^V_0)^4\right] = {\sigma'}^2$.

Definition 4.1. *Define the NPK matrix to be* $H_{\Theta^F_0} \stackrel{def}{=} \Phi^\top_{\Theta^F_0}\Phi_{\Theta^F_0}$.

Theorem 4.1. *As* $w \rightarrow \infty$*,* $K_{\Theta^{DGN}_0} \rightarrow d\sigma^{2(d-1)} H_{\Theta^F_0}$.

From pervious results, **??**, if follows that as $w \rightarrow \infty$, the optimisation and generalisation properties of the fixed NPF learner can be tied down to $H_{\Theta^{\mathrm{F}}_0}$ (treating $d\sigma^{2(d-1)}$ as a scaling factor).

4.1 Properties of NPK

Definition 4.2. *For input examples* $s, s' \in [n]$ *define*

1. $\tau_\Theta(s,s',l) \stackrel{def}{=} \sum_{i=1}^{w} G_{x_s,\Theta}(l,i) G_{x_{s'},\Theta}(l,i)$ *be the number of activations that are "on" for both inputs* $s, s' \in [n]$ *in layer l.*

2. $\Lambda_\Theta(s,s') \stackrel{def}{=} \Pi_{l=1}^{d-1} \tau_\Theta(s,s',l)$.

For a given example $s \in [n]$, $\Lambda_\Theta(s,s)$ is a measure of the total number of active paths for that input example, and for different input examples $s, s' \in [n]$ it is a measure of total number of paths that are active for both examples $s, s' \in [n]$. Thus, $\Lambda_\Theta \in \mathbb{R}^{n\times n}$ is the correlation matrix that measures the amount of overlap the active sub-networks.

Lemma 4.1. *Let* $\Sigma \in \mathbb{R}^{n\times n}$ *be the* $n \times n$ *input Gram matrix with* $\Sigma(s,s') = \langle x_s, x_{s'}\rangle, s, s' \in [n]$*. It follows that* $H_\Theta = \Sigma \odot \Lambda_\Theta$*, where* $\odot$ *stands for the Hadamard product.*

Note that Σ is a constant, while Λ_Θ is learnt during training, and from Theorem 4.1 it follows that:

Claim 1: The information in the gates of a DNN is captured in its active sub-networks.

5 Experiments

In this section, we experimentally verify the following claim.

Claim 2: Dynamics of the gates, i.e., NPF learning is key for generalisation.

Experimental Setup: We used standard datasets namely MNIST, CIFAR-10, and CIFAR-100, with categorical cross entropy loss. We used stochastic gradient descent (SGD) and *Adam*. In the case of SGD, we tried constant step-sizes in the set $\{0.1, 0.01, 0.001\}$ and chose the best. In the case of Adam the we used a constant step size of $3e^{-4}$. In both cases, we used batch size to be 32. We used a fully connected (FC) DNN with $(w = 128, d = 6)$ for MNIST.To train CIFAR-10, we used *Vanilla-Convolutional* Network (VCONV) without pooling, residual connections, dropout or batch-normalisations, and is given by: input layer is $(32, 32, 3)$, followed by convolution layers with a stride of $(3, 3)$ and channels 64, 64, 128, 128 followed by a flattening to layer with 256 hidden units, followed by a fully connected layer with 256 units, and finally a 10 width soft-max layer to produce the final predictions. To train CIFAR-10, we also used a GCONV which is same as VCONV with a *global-average-pooling* (GAP) layer.

1. **DNPFL:** Here, we use $\chi^g = \chi_r$, and $G_{x,t}(l) = \gamma_{sr}\left(q^g_{x,t}(l)\right)$. We initialise and train both Θ^{F}_t and Θ_t with $\hat{y}^v_t(x_s)$ as the output node. The use of soft-ReLU makes it straightforward for the feature gradients to flow via the gating network. The GD dynamics is given in the third column from left in **??**.

2. **Random FixedNeural Path Feature (RFNPF)**: Here, we use $\chi^g = \chi_r$, and $G_{x,t}(l) = \gamma_r\left(q^g_{x,t}(l)\right)$. Also, the weights of the gating network are initialised at random, however, there are made non-trainable, i.e., $\Theta^{\mathrm{F}}_0 = \Theta^{\mathrm{F}}_t, \forall t \geq 0$. There are two possible initialisations namely i) *independent initialisation* (II), i.e., Θ^{F}_0 and Θ_0 are statistically independent, and ii) *dependent initialisation* (DI), i.e., $\Theta^{\mathrm{F}}_0 = \Theta_0$, a case which mimics the NPFs and NPVs of a standard DNN with ReLU activations. After initialisation, Θ_t is trained with $\hat{y}^v_t$ as the output node.

Arch	Optimiser	Dataset	FRNPF (II)	FRNPF (DI)	DNPFL	FLNPF	ReLU
FC	SGD	MNIST	95.85 ± 0.10	95.85 ± 0.17	97.86 ± 0.11	97.10 ± 0.09	97.85 ± 0.09
FC	Adam	MNIST	96.02 ± 0.13	96.09 ± 0.12	$\mathbf{98.22 \pm 0.05}$	$\mathbf{97.82 \pm 0.02}$	$\mathbf{98.14 \pm 0.07}$
VCONV	SGD	CIFAR-10	58.92 ± 0.62	58.83 ± 0.27	63.21 ± 0.07	63.06 ± 0.73	67.02 ± 0.43
VCONV	Adam	CIFAR-10	64.86 ± 1.18	64.68 ± 0.84	$\mathbf{69.45 \pm 0.76}$	$\mathbf{71.4 \pm 0.47}$	$\mathbf{72.43 \pm 0.54}$
GCONV	SGD	CIFAR-10	67.36 ± 0.56	66.86 ± 0.44	$\mathbf{74.57 \pm 0.43}$	$\mathbf{78.52 \pm 0.39}$	$\mathbf{78.90 \pm 0.37}$
GCONV	Adam	CIFAR-10	66.42 ± 0.44	66.81 ± 0.75	$\mathbf{77.12 \pm 0.19}$	$\mathbf{79.28 \pm 0.13}$	$\mathbf{80.32 \pm 0.13}$

Table 2: Shows the training and generalisation performance of various NPFs.

3. **Learned Fixed Neural Path Feature (LFNPF)**: Here, we use $\chi^g = \chi_r$, and $G_{x,t}(l) = \gamma_r\left(q^g_{x,t}(l)\right)$. First we train a standard DNN with ReLU activations parameterised by $\bar{\Theta}_t \in \mathbb{R}^{d_{net}}$(whose architecture is identical to the value/ gating network) for T_L epochs. We copy the weights onto the gating network, i.e., $\Theta^{\text{F}}_0 = \bar{\Theta}_{T_L}$, which are then made non-trainable. We then initialise and train Θ_t with $\hat{y}^v_t$ as the output node.

We now discuss the results in Table 2, and the results of two more experiments.

1. **FRNPFs** do generalise, they are outperformed by DNPFL, FLNPF, and standard ReLU all of which involve NPF learning. While the DNPFL, and FLNPF are new in the paper, the fact that fixed random NTFs generalise poorly than DNNs with ReLU activations has been reported in **?**. In best case scenarios, the pure NTK based method performs poorly than standard ReLU by approximately 5.5% (see Table 1 in **?**) in CIFAR-10, and the random NTFs from a finite DNN performs poorly than the infinite width limit NTK by approximately 5% (see last row of Table 2 in **?**). We also note that initialisations II and DI did not show much difference in performance.

2. **NPF learning improves generalisation:** Models with NPF learning namely DNPFL, FLNPF, and standard DNN with ReLU, perform better than FRNPFs. It is very interesting to note that FLNPF perform almost as well as the standard DNNs with ReLU activations.

3. **Role of GAP:** In **??** discussed how ConvNets with GAP or $\max$-pooling have translation invariance property, and in **??** we showed that the NPK has a component that is translation invariant. In our experiments, and also in those of **?**, adding the GAP layer gives a performance improvement of approximately 10%.

4. **Addressing the research gaps:** The gap in the generalisation performance of fixed NPFs and that of DNN with ReLU is continuous. The gap gradually closes as we move from FRNPFs to FLNPFs. We trained a DNN with ReLU (parameterised by $\bar{\Theta}$) for 60 epochs, and we obtained 6 different NPFs from these weights at various *stages*, i.e., stage 1: $\bar{\Theta}_{10}$, stage 2: $\bar{\Theta}_{20}$, stage 3: $\bar{\Theta}_{30}$, stage 4: $\bar{\Theta}_{40}$, stage 5: $\bar{\Theta}_{50}$, stage 6: $\bar{\Theta}_{60}$. We trained with these 6 different fixed NPFs by setting $\Theta^{\text{F}}_t = \Theta^{\text{F}}_0 = \bar{\Theta}_{10\times i}, i \in [6]$ and training the Θ_t in the DGN. The results are shown in the leftmost plot in Figure 2, where, the performance of FLNPF through stage 0 (i.e., random/no learning) to stage 6 (full learning) is shown. The performance of convolutional NTK (CNTK) **?** (77.43%) is given by the orange dotted line. The result of Theorem 4.1 and the performance of FLNPF through stages together indicate that the gap in the performance of the CNTK and CNN (with ReLU) is due to the presence and absence of NPF learning and perhaps not because of finite vs infinite width as suggested by **?**. Note that the best performance of CNN with GAP in **?** is 83.30%, and our model gives only 80.3%, a difference we attribute to the difference in the two models.

Observation: Almost all information is stored in the gates of a DNN.

5. **NPF learning during training:** We consider "Binary"-MNIST data set with two classes namely digits 4 and 7, with the labels taking values in $\{-1, +1\}$ and squared loss. We trained a standard DNN with ReLU activation ($w = 100$, $d = 5$). Let $\widehat{H}_t = \frac{1}{trace(H_t)} H_t$ be the normalised NPK matrix. For a subset size, $n' = 200$ (100 examples per class) we plot $\nu_t = y^\top(\widehat{H}_t)^{-1} y$, (where $y \in \{-1, 1\}^{200}$ is the labeling function), and observe that ν_t reduces as training proceeds (see **??**). Note that, $\nu_t = \sum_{i=1}^{n'} (u_{i,t}^\top y)^2 (\hat{\rho}_{i,t})^{-1}$, where $u_{i,t} \in \mathbb{R}^{n'}$ are the orthonormal eigenvectors of $\widehat{H}_t$ and $\hat{\rho}_{i,t}, i \in [n']$ are the corresponding eigenvalues. Since $\sum_{i=1}^{n'} \hat{\rho}_{i,t} = 1$, the only way ν_t reduces is when more and more energy gets concentrated on $\hat{\rho}_{i,t}$s for which $(u_{i,t}^\top y)^2$s are also high.

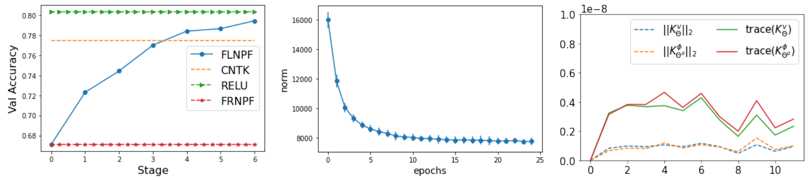

Figure 2: Dynamics of Learning

6. **Decoupled NPF learning (DNPFL)** also yields good generalisation performance. This paves an interesting future direction: in this case the NTK is given by $K_{\Theta,\Theta^{\mathrm{F}}} = K^v_{\Theta} + K^{\phi}_{\Theta^{\mathrm{F}}}$, and the problem can be simplified by studying K^v_{Θ} and $K^{\phi}_{\Theta^{\mathrm{F}}}$ separately. As a start, in the case of MNIST, we compared K^v_{Θ} and $K^{\phi}_{\Theta^{\mathrm{F}}}$ using their trace and Frobenius norms, and we see that K^v_{Θ} and $K^{\phi}_{\Theta^{\mathrm{F}}}$ are in the same scale, which is perhaps pointing to the fact that both K^v_{Θ} and $K^{\phi}_{\Theta^{\mathrm{F}}}$ are equally important for obtaining good generalisation performance.